

Chapter Five

Synthesis and Modeling

5.1 Overview

Despite near-term advances in in situ measurements and remote sensing, observations of carbon in the ocean and atmosphere alone will remain too sparse to adequately characterize the time-space variability of the global carbon cycle and the net carbon fluxes among reservoirs. Numerical modeling including data assimilation will therefore play a pivotal role in the synthesis and interpretation of carbon cycle data. Modeling considerations should also be incorporated from the beginning in developing a global observational strategy, with particular focus on the network design for sampling and timely public access to data. This research is essential to help answer the first fundamental question raised by the U.S. Carbon Cycle Science Plan (CCSP), namely, what has happened to the carbon dioxide already emitted by human activities? The second basic question raised by this plan is, what are the likely future trends in atmospheric CO₂ concentrations? This question can be answered only with prognostic models. Improving such models must therefore be one of the principal goals of carbon cycle research over the next decade.

Three classes of models are envisioned here as essential to a global ocean-atmosphere-land carbon cycle observing strategy.

1. Prognostic (forward) atmospheric circulation/transport models and oceanic circulation/biogeochemistry models.
2. Diagnostic (inverse) versions for the same types of atmosphere and ocean models.
3. Data assimilation models for atmosphere and ocean biogeochemistry.

Two other categories of models are also discussed here and are essential from a broader perspective on carbon cycle research.

1. Land-surface biogeochemical models.
2. Comprehensive (coupled) ocean-atmosphere-land climate and carbon cycle models.

Significant progress can be achieved in carbon cycle modeling over the next 5–10 years. First, the development and evaluation of biogeochemical models are grounded by field data at a fundamental level, and the recent and ongoing expansions of the observational base for carbon will accelerate numerical modeling. Second, data assimilation is emerging as a new and powerful tool in biogeochemistry, providing the tools to combine data and

models into a coherent description of the carbon system. Third, coupled carbon cycle models are maturing to a point where we can study the dynamics of the Earth system as a whole.

During the 5-year ramp-up phase, the synthesis and modeling component should include the following research foci and infrastructure elements that are common to all three observing domains:

- Augmented/new carbon data centers to undertake or coordinate the compilation, quality control, and distribution of in situ and remote-sensing data relevant to the carbon cycle, as well as derived synthesis products (e.g., surface fluxes and assimilation fields) produced by the research community.
- Process and inverse modeling studies to design optimal sampling networks and assess the utility and tradeoffs among existing and emerging measurement and platform technologies.
- Ongoing development and improvement of atmospheric transport and oceanic circulation and biogeochemical models used to diagnose carbon sources and sinks; direct evaluation of simulations against observations must be integral to the model development effort.
- Comparison and reconciliation of independent estimates of regional air-sea CO₂ fluxes from direct observations, atmospheric inversions, and oceanic inversions; this central effort compares results from all three observing domains.
- Hindcast simulations and data synthesis of the ocean/atmosphere/land carbon cycle variability over the recent historical period (1950s–present) using atmospheric reanalysis products and ocean state estimations.
- Pilot data assimilation studies to investigate the methods, data needs, and general feasibility of ocean/atmosphere/land carbon data assimilation systems. In the longer term, synthesis and modeling must evolve to full data assimilation systems to provide ongoing evaluations of carbon sources and sinks and the underlying mechanisms.
- High-resolution physical circulation and biogeochemical models for specific process studies and to provide context for regional campaigns and field experiments.
- Prognostic coupled climate model development and simulations to improve projections of the carbon cycle’s future evolution under various scenarios for emissions, land use, and other areas.

The carbon cycle is embedded in the physical climate system; close collaboration with the weather, physical oceanographic, and climate communities is imperative, both for observational systems and modeling, and will be synergistic and mutually beneficial. Similar strong linkages must be established with the terrestrial carbon cycling community. The remainder of this

chapter covers the general synthesis and modeling elements for an ocean-atmosphere observing system and topics that relate more specifically to the other chapters of this report (on observing CO₂ in the atmosphere, surface ocean, and the ocean interior). This chapter's recommendations on modeling and synthesis are more general than those in the observation chapters, and cost estimates for recommended activities have been omitted here.

5.2 Recommendations

5.2.1 Carbon data management and distribution

The proposed carbon data center(s) would act as the collection point for the various types and levels of data streams. For many types of data, particularly for those collected via spaceborne platforms, such centers are already in existence and do not need to be duplicated. However, for many other observations—for example, those associated with the rapidly increasing number of underway pCO₂ data and airborne CO₂—such a center(s) needs to be established and supported. The data synthesis at these sites might include quality control procedures beyond the initial quality control at the level of individual measurements and observational networks. This includes, for example, investigating the internal consistency of the data as well as testing for long-term data precision and accuracy. High priority should also be given to fully documenting the various data products and streams (metadata). The data centers would be responsible for publicly distributing the data electronically (most likely via the web) in a timely fashion, following the models set up by CDIAC, JGOFS, WOCE, and others. Data and funding policies need to be established at the program's beginning to ensure prompt data submittal and release. Finally, data centers would serve as repositories and distribution points for synthetic data products (e.g., flux estimates, interpolated fields, assimilation output) developed as part of the project.

5.2.2 Sampling network design

The creation of a global carbon cycle observing system faces daunting challenges, among them the wide range of relevant time-space scales, from synoptic to decadal, and from mesoscale and regional to basin/continental scale. Fortunately, a set of relatively new sensor, sampling, and platform technologies (e.g., airborne sampling and autonomous sensors on moorings and drifters) are greatly expanding our view of atmospheric and oceanic biogeochemistry. Nevertheless, the optimal mix of these new and more traditional methods for an improved sampling network are not well known. A number of atmospheric inversion studies using relatively coarse resolution transport models have explored the impact on surface carbon flux estimates of expanding the ground-based air-sampling network and/or adding airborne and satellite measurements. More work is likely required, however, at fine spatial resolution and incorporating more sophisticated dynamics (e.g., diurnal cycle, planetary boundary layer) to refine surface CO₂ flux estimates. For

the ocean, preliminary sampling requirements have been defined for surface $p\text{CO}_2$ and carbon inventory sections using statistical methods (see Appendix D, Appendix E, and Chapter 4). Again, more detailed study using formal inverse techniques and high-resolution process models is warranted, particularly as new data sets become available.

5.2.3 Ocean and atmosphere prognostic model—data evaluation

Focused research on forward or prognostic atmospheric transport and ocean biogeochemical models is required to better quantify surface CO_2 fluxes, develop a fundamental understanding of processes controlling those fluxes, and improve future climate projections. Particular emphasis should be placed initially on physical circulation, because carbon is redistributed horizontally and vertically by constantly varying atmospheric and oceanic transport. Therefore, synthesis of observations and interpretation of data require adequate representation of advection and mixing as well as their variations. Atmospheric and oceanic constituents have source and sink distributions and lifetimes different from temperature, humidity, salinity, and other traditional physical circulation parameters. The simulation of tracer distributions therefore demands different strengths and tolerates weaknesses in general circulation models (e.g., TransCom, the Ocean Carbon Model Intercomparison Project [OCMIP]).

In particular, the IGBP-GAIM TransCom and OCMIP intercomparisons reveal large discrepancies in model simulations of the vertical and horizontal structure of tracers in both atmosphere and ocean. These discrepancies result largely from uncertainties in the representation of subgrid processes in the models, and the required improvements in the models are often parallel in atmospheric and oceanic models. Examples include, but are not limited to, diurnal and seasonal dynamics of the atmospheric planetary boundary layer and the oceanic mixed layer; mixing and transport of tracers by clouds and deep/intermediate water formation; flow over orography and boundary currents; and diapycnal and isopycnal mixing.

The OCMIP intercomparison has also begun to evaluate the biogeochemical components of ocean models using the rich database from the JGOFS/WOCE global CO_2 survey (e.g., nutrients, DIC, oxygen). The treatment of biology in these models is woefully crude, however, and a new round of model-data evaluation is called for, one that incorporates biology in ways intended to better predict or describe the sea surface $p\text{CO}_2$ field based on mechanistic principles.

5.2.4 Reconciliation of air-sea CO_2 flux estimates

Air-sea fluxes of CO_2 can be derived in three independent ways: inversion of atmospheric CO_2 concentrations using atmospheric transport models (ATMs), inversion of interior oceanic carbon system observations using oceanic circulation/biogeochemistry models, and direct in situ observation of air-sea $\Delta p\text{CO}_2$ and wind speed or sea surface roughness, proxies for gas

transfer velocity. Confrontation of these independent estimates would challenge both the models and measurements. Reconciling these independent estimates would provide confidence in the regional carbon sinks inferred from the atmospheric CO₂ data. The construction and intercomparison of these estimates represents the intersection of the three axes of the entire observation program, and hence is a major focus.

Inverse or diagnostic models are routinely used to estimate air-sea fluxes of CO₂ (and other biogeochemical gases such as O₂) from the atmospheric surface sampling network data. The atmospheric transport research community has a rich history in this area, and inverse techniques have the advantage of quantifying regional (subbasin to basin-scale) flux magnitudes as well as the associated uncertainties. The resulting model-generated products provide the input needed for scientific and political assessments and the initial conditions for short-term and long-term predictions using prognostic models. Similar methods can be applied to ocean circulation models and subsurface carbon observations, but work on these applications is just beginning. The more traditional, direct oceanic air-sea flux approach requires spatial and temporal interpolation of the sparse in situ pCO₂ data and estimates of air-sea gas transfer from wind speed (as determined by atmospheric analysis, satellite scatterometry, etc.) and/or satellite surface roughness. The most straightforward interpolation methods involve statistical objective analysis. The next level of sophistication incorporates information from more densely sampled and/or remotely sensed ocean properties (e.g., sea surface temperature and salinity, ocean color) using either empirical or theoretical relationships (full data assimilation is discussed in more detail below).

5.2.5 Hindcast simulations

The Earth's climate exhibits significant subannual, interannual, and decadal variability across a range of spatial scales from regional to global, with much of the nonseasonal signal associated with regional climate modes such as the El-Niño/Southern Oscillation (ENSO), North Atlantic Oscillation (NAO), Antarctic Circumpolar Wave, and the like. The observed growth rate of atmospheric CO₂ contains considerable temporal variability on similar scales, which can be partitioned with inverse techniques into land and ocean contributions based on spatial patterns and atmospheric $\delta^{13}\text{C}$ and O₂/N₂ data. Even more information can be derived by examining the spatial and temporal variability patterns of marine and terrestrial ecosystems. Natural climate variability offers a ready-made set of perturbation and/or sensitivity studies that can clarify the physical and biological mechanisms governing carbon cycle dynamics. In addition to replicating the large-scale geographic patterns of the mean state and seasonal cycle, particular emphasis should be placed on evaluating the ability of prognostic models to hindcast the atmosphere/ocean/land carbon cycle and biogeochemical responses to interannual to decadal natural variability. The experience gained from this research will feed into the continued development and improvement of prognostic models for simulating the future evolution of carbon dioxide under a range of emissions scenarios.

5.2.6 Data assimilation

Data assimilation models have roots in numerical weather prediction, in which synoptic meteorological observations are continuously fed into numerical weather models to produce a global, gridded, synoptic description of the atmospheric circulation every 4 or 6 hours. The assimilation models thus merge diverse data streams into a single framework, interpolating and extrapolating observations spatially and temporally, and imposing internal consistency among the various parameters in the analyzed products.

The development of assimilation models will contribute centrally to the formulation of a strategy for constraining regional carbon budgets. It is crucial to use a diversity of approaches and models to derive and reconcile these estimates, and data assimilation provides a coherent framework for conducting such work. The results from the atmospheric inversions also should be evaluated with the fluxes predicted from maturing terrestrial carbon simulations, to assess flux magnitudes and patterns, and to isolate the physical and biogeochemical driving factors.

To accomplish this task, data assimilation models must be expanded to incorporate carbon observations, including related tracer and remote-sensing data. The initial focus will likely be on assimilating atmospheric (or ocean) CO₂ concentration data alone, but with time more integrated systems will evolve that fold in biological data streams, such as satellite-derived terrestrial vegetation indices and surface ocean color. Data assimilation models already capture much of the variability in the physical climate system on synoptic to interannual timescales, and so the assimilated carbon products would be dynamically consistent with the temporally evolving atmospheric and oceanic circulation. Additional data products would include optimal estimates of all the carbon state variables and fluxes resolved in the numerical simulation (e.g., net community production and surface CO₂ fluxes). As emphasized below, the infrastructure costs of full-scale, numerical data assimilation are large, and it is presently unclear whether the best course would be to incorporate carbon into the (mostly) operational atmosphere and ocean data assimilation efforts or to develop a parallel data assimilation system more specifically tailored for carbon cycle studies.

Assimilation of ocean carbon observations into atmosphere and ocean models is a new area of research, and an initial research phase is strongly encouraged before making the transition toward a more operational mode. In the research phase, a diversity of approaches and numerical models must be used. The intercomparison of these methods and models and assessment of the realism of the “analyzed” carbon products will challenge and accelerate the development of the biogeochemical parameterizations. The meteorological community has an extensive history with atmospheric data analysis and assimilation models, which form a core component of the operational weather forecasts (e.g., NCEP, ECMWF). These techniques have also been expanded to seasonal and interannual climate prediction issues (e.g., ENSO), incorporating coupled upper ocean, atmosphere, and land physical models and satellite remote-sensing data (e.g., the NASA Goddard DAO assimilations). The CLIVAR program and Global Ocean Data Assimilation

Experiment (GODAE) have attempted to elevate global ocean state estimation from its current experimental status to a quasi-operational tool for climate research and prediction. A number of hindcasting ocean state estimation projects are also underway (e.g., ECCO—Estimating the Circulation and Climate of the Ocean). The development of a carbon data assimilation program should build on and leverage collaborations with NOAA, CLIVAR, GODAE, and NASA.

5.2.7 Prognostic (forecast) simulations

Coupled carbon and climate models are needed for projecting the influence of terrestrial and oceanic processes on the rate of atmospheric CO₂ growth and climate change; they are also needed to identify carbon/biogeochemistry metrics that may be early (fast response) signals of slow climate change. Coupled models will also serve as the framework for integrated global carbon cycle data assimilation. The United States needs to develop the capability for a comprehensive climate system modeling program built on high-end, global models that cover a number of areas:

- The coupling of all components of the climate system.
- All processes that determine the composition of CO₂ and other radiatively and chemically important trace constituents in the atmosphere.
- Future climate change over the next several centuries under a range of social, political, and economic scenarios.
- A systematic set of tracers and diagnostics that can be used to evaluate the model performance for regional assessment.

The carbon cycle must be an integral component of such an effort, which must build on and leverage process-level research on the physical, chemical, and biological mechanisms governing the climate system. One critical source of process-level information is the large-scale tracer observations that, interpreted with models, reflect carbon fluxes and their relation to forcing.

5.2.8 Modeling studies for atmospheric CO₂

As outlined in the chapter on needed atmospheric observations, there is much more information on continental and basin scale carbon exchange in even the current atmospheric data stream than we are able to extract with current transport models. As the observing system is expanded to include more continental locations and satellite derived CO₂ fields, models will increasingly be called on to quantify CO₂ surface flux information from the atmospheric concentration data on finer regional scales. There are three basic synthesis and modeling needs specific to the atmospheric observation component:

- Improve atmospheric tracer model representation of the synoptic wind field, diurnal cycle, and vertical mass transport.
- Incorporate carbon data assimilation into global atmosphere models.

- Develop high-resolution mesoscale atmosphere-land carbon cycle models to support regional field campaigns.

Improve tracer model representation of the synoptic wind field, the diurnal cycle, and vertical mass transport to better resolve the high-frequency variability observed in continuous measurements and observations in continental interiors

Most atmospheric observations to date have focused on remote background locations, which could be analyzed with the coarse-resolution atmospheric transport derived from GCMs. Newer stations in continental locations are much more strongly influenced by local to regional sources and sinks. Terrestrial fluxes are strongly variable in both space and time, as is atmospheric transport over land. Taken together, this variability in fluxes and transport produces much “noisier” time series of tracer concentration at continental observing locations than in the remote marine boundary layer. Current sampling protocols are dominated by discrete sampling, providing a single measurement from a highly variable concentration field. Such measurements are only representative when they are averaged over many samples, for example, as monthly means. Present inverse modeling studies optimize monthly mean concentration fields simulated by global ATMs over grid cells of more than 10^5 km² through depths of hundreds to thousands of meters. Data used in these inversions are typically monthly mean concentrations calculated from discrete samples. The analysis therefore inappropriately compares simulated mass-weighted means sampled continuously to the mean of a handful of point measurements taken from a continuously varying field.

More information is in principle extractable from highly variable concentration data, but requires accurate knowledge of the upstream trajectory of the air being sampled. Many of the current models being used for inversion studies do not even use “real” winds, relying on correct simulation of the climatological transport operator to optimize a fit to the climatology of observed CO₂. Some models do calculate tracer transport using analyzed winds, produced by weather forecasting centers. Wind fields generated in this way are also model simulations, though they have been made consistent with observations in an optimal way through data assimilation methods. Unfortunately, these wind fields are largely unconstrained by data in some areas of the world with few soundings (notably large areas of the Pacific and Southern Oceans). In addition, forecast and analysis centers typically do not archive vertical mass transport due to unresolved physical processes such as moist convection and turbulence. In ATMs driven by analyzed winds, these mass fluxes are usually estimated independently, using algorithms that are different than the ones used in the “parent” forecast model. The resulting inconsistency in transport between the resolved advection (estimated by the forecast model) and the vertical mass fluxes (estimated by the physical parameterization in the off-line ATM) reduces the realism of the simulated tracer field.

Making the most out of future observations that include high-frequency time series, such as records from continuous analyzers on tall towers, will

require not only accurate transport by “real winds,” but also accurate simulation of vertical structure. Meeting this goal will require dedicated efforts to advance the state of the art of simulating diurnal variations in surface ventilation and entrainment at the top of the planetary boundary layer and the effects of vertical transports in cumulus clouds. ATMs used for inversion of continuous records may require high vertical resolution near the surface, but the height of the top of the planetary boundary layer varies from 100 m under very stable conditions to several kilometers under strongly convective conditions. The challenge then is to resolve strong tracer gradients and entrainment processes at whatever height they occur in the lower troposphere. Of course, the representation of planetary boundary layer entrainment and cumulus convection is also of paramount importance in weather and climate modeling, and it is the subject of very active research in the physical climate community. Models used for numerical weather prediction are already using advanced physical parameterizations and running on grids of as small as 50 km (or equivalent spectral resolution).

High time-resolution flux estimates may be obtained from continuous, high-frequency data through the use of realistic transports obtained from operational weather analyses. The most serious impediment to this kind of analysis today is the lack of subgrid-scale mass fluxes. A top priority for inverse model development should be to obtain both winds and convective transports from Numerical Weather Prediction (NWP) centers at the highest possible resolution, preferably on an hourly time step. This achievement will allow analysis of actual cases from continuous analyzers as opposed to time means. Shifts in concentration during frontal passage, wind shifts, or other weather events would then become part of the signal in the inversion, rather than being treated as noise. Weather analysis and reanalysis products have typically been provided on a 6-hour basis, and subgrid-scale mass fluxes have not been included. Extending these products to hourly time resolution and including parameterized transports would dramatically increase data storage and transmission requirements. But recent advances in both areas have exceeded Moore’s Law, and such increases are now both technically feasible and economical. Realistic model transports at high temporal and spatial resolution will enable inversion analysis to move toward direct assimilation of concentration data for surface flux estimation. Assimilation methods have already been explored using existing ATMs (Bruhwiler *et al.*, 1999; Dargaville *et al.*, 2000; Rayner *et al.*, 2000). Applying these methods to highly resolved transports from a new generation of reanalysis products would substantially improve flux estimates and exploit the new information being provided from continental observations. These improvements could be obtained in the next 2 years and should be strongly encouraged, but will require significant effort and resources from one or more NWP centers.

Develop techniques and methods for carbon data assimilation into global atmospheric models

Real-time assimilation of satellite and in situ CO₂ estimates in operational weather forecasting would provide an ideal framework for estimation of re-

gional surface CO₂ fluxes by mass balance. Carrying tracer concentrations as a prognostic variable in the assimilation provides strong constraints from the “memory” in the atmosphere and would reduce artificial noise from poorly constrained CO₂ retrievals. Assimilated CO₂ concentrations in operational NWP models would produce fully populated, global gridded data, filling the gaps left by clouds, yet remaining optimally consistent with existing observations. Correct knowledge of atmospheric CO₂ also has recently been shown to improve the retrieval of temperature profiles from infrared spectroscopy, reducing forecast initialization error by as much as 1 K over some regions (Engelen *et al.*, in press). Achieving this goal will require the commitment of operational NWP centers and their sponsors. Such a program is technically feasible and could be implemented as early as 2002, when satellite CO₂ estimates begin to be available from the Atmospheric Infrared Sounder (AIRS) aboard EOS-Aqua. The operational centers (for example, NCEP, ECMWF, and NASA DAO) have the requisite human resources and skill, computing infrastructure, and data-handling capability, but the centers have correctly argued that such analyses are beyond their weather forecasting mandate. Significant new resources would be required to accomplish routine CO₂ data assimilation, yet the scientific return is potentially enormous, especially later in the decade when higher quality global satellite products are expected to become available.

Spaceborne CO₂ data alone, however, will not solve all of the problems, and a major need in the next 5 years will be to analyze possible bias in trace gas products derived from satellite retrievals. This will entail substantial field sampling programs (see section on atmospheric observations), but also may require models to extrapolate data into unobservable “gaps.” Sensors relying on reflected sunlight, for example, will see only daytime conditions, which are likely to have systematically lower CO₂ concentrations over vegetated land than the true mean. Similarly, almost any spaceborne estimate of CO₂ concentration will be biased to clear sky conditions, which may result in small but systematic errors over time. To counter these biases, models used for data analysis, assimilation, and flux estimation will need better parameterizations of high frequency surface flux and vertical mixing variability, for example, accounting for diurnal cycles over land.

Develop high-resolution mesoscale atmosphere-land carbon cycle models to support regional field campaigns

In addition to developing and improving *global* ATMs for inverse calculation of surface carbon fluxes by data assimilation, there is a need for model development in support of regional field campaigns. Such campaigns (e.g., BOREAS, LBA, COBRA, and SAFARI2000) are an important test of the ability of simulation models to scale from locally observable processes (flux tower scale) to larger regions. They provide an opportunity to apply the same sort of mass-balance constraint on such upscaled models that can be obtained at continental scale through inverse modeling, but at much finer scales for specific cases. Aircraft sampling can strongly constrain predictive models of carbon and other trace gas fluxes, but only if trajectories are

known in considerable spatial and temporal detail for the actual flight days and times. Even the very best global meteorological data analysis products have insufficient resolution to be very useful for this purpose. Mesoscale atmospheric models can be driven from globally gridded data, with “nests” down to 1 km or finer for this purpose, and operational analysis and forecasts from such models can therefore be very useful in support of field campaigns. Such models can resolve features of circulation and transport, for example moist convection and entrainment at the top of the planetary boundary layer, that must be parameterized in global models. Case studies from field campaigns in which fine-scale analyses are well constrained by observations can also be used as test beds for improved parameterizations of these processes in global models.

Most mesoscale atmospheric models in current use can be run from analyzed fields at larger scale and are thus already available for use in field campaigns. Very few, if any, however, are coupled to ecophysiological process models that predict spatial and temporal variations of photosynthesis and respiration. Intensive field campaigns, such as those conducted by CarboEurope and the proposed North American Carbon Experiment, would be excellent tests of such models. As computer power increases, it will be possible to simulate coupled interactions among weather, hydrology, and biogeochemistry at scales of a few kilometers over continental-sized regions for periods of up to a year. Such a simulation would be very expensive to run, but could be tested quite rigorously against data from surface, airborne, and spaceborne platforms. These tests, which would provide significant insight, algorithm development, and even code for the development of the global coupled assimilation models, could be accomplished in the next 5 years. By the end of the decade, these fine-scale models would likely merge with the more ambitious global coupled models and be run routinely at global scale on grids of 10 km or less.

5.2.9 Modeling studies for upper ocean physics/biogeochemistry and sea surface pCO₂

There are four basic synthesis and modeling challenges specific to the surface CO₂ observations component:

- Improve quantification of the time/space correlation scales for surface pCO₂, surface air-sea CO₂ flux, and other relevant physical and biogeochemical properties as the basis for the design of sampling programs.
- Relate observed and historical patterns and variability in pCO₂ and ancillary tracers (TCO₂, TA, O₂, nutrients, isotopic composition of these species) to the underlying biological and physical mechanisms.
- Develop empirical and mechanistically based numerical methods for extrapolating in situ pCO₂ data and air-sea flux estimates to basin-scale.
- Initiate surface ocean color and pCO₂ data assimilation studies.

The objectives are of course related in that improved understanding of the governing dynamics provides a more rigorous basis for time/space extrapolation and data assimilation.

Quantify the time/space correlation scales of surface pCO₂, surface air-sea CO₂ flux, and other relevant physical and biogeochemical properties via synthesis of in situ and remotely sensed data and high-resolution process models

Appendices E and F present preliminary sampling density requirements for a surface pCO₂ observing system based on statistical analyses of existing underway pCO₂ and time-series data. These estimates need to be refined over the first 5 years of the program using a combination of new surface data from instrumented moorings, drifters, and volunteer observing ship lines and directed modeling studies. An important question involves identifying the degree to which pCO₂ is correlated with the gas exchange coefficient, which might result, for example, from strong winds and the ensuing vertical mixing. The key is to better characterize the relevant time and space correlation scales for surface pCO₂, air-sea CO₂ flux, and other biogeochemical fields. Time/space scales are fundamental to basin-scale extrapolation as well (see below). An iterative procedure is envisioned whereby new scale estimates are applied and the resulting skill of basin extrapolations (compared, for example, to independent data withheld from the analysis) is used to guide revised scale estimates and sampling requirements.

Surface pCO₂, air-sea CO₂ flux, and ocean biology vary on a wide range of scales driven primarily by ocean/atmosphere physics: synoptic events (e.g., storms), submesoscale fronts, mesoscale eddies, and gyre circulation and climatic modes. Present measurement technologies typically limit the high-resolution sampling of pCO₂ to one dimension, either in space (e.g., a VOS underway line) or time (e.g., a moored time-series record). In a research mode, it is possible to make two-dimensional and partial three-dimensional surveys with dedicated seasoar surveys along a grid of transect lines. Analyses of satellite surface fields of physical properties (e.g., sea surface temperature, sea surface height) and biological properties (e.g., ocean color) suggest that the mesoscale (roughly 10–100 km) is a dominant scale of variability.

Eddy-resolving numerical models can provide a more complete picture of the time-evolving three-dimensional fields of the upper ocean and the relationship of pCO₂ to remotely sensed properties. A number of eddy-resolving biogeochemical process models have been developed (e.g., McGillicuddy and Robinson, 1997; Mahadevan and Archer, 2000). The Mahadevan and Archer work is particularly interesting because it uses idealized tracers to show the relationship between time and space scales across the submesoscale and mesoscale, more slowly evolving tracers having longer space scales. Eddy-resolving, basin-scale ecosystem models have also been constructed (e.g., Oschlies and Garçon, 1999), but some caution is warranted because very high resolution ($\sim 1/10^\circ$) is required to properly capture the statistics of the eddy field and the eddy-mean flow interaction (Smith *et al.*, 2000). Some

encouraging, very simple biogeochemical studies are being conducted on this scope (McGillicuddy *et al.*, in preparation). Even higher resolution submesoscale processes may also be important. Carbon system dynamics need to be incorporated into these classes of models to explore the high-frequency space/time variability in surface pCO₂.

Develop improved empirical and mechanistically based methods for extrapolating in situ pCO₂ data and air-sea flux estimates to basin scale

At the simplest level, the basin-scale extrapolation problem can be viewed as one of objectively analyzing a sparsely sampled field in space and time. The Takahashi *et al.* (1997, 1999) climatology, for example, is constructed using inhomogeneous and anisotropic correlation scales derived in part from the surface circulation field of an ocean general circulation model. Additional information can be incorporated using empirical relationships with satellite sea surface temperature, ocean color, and climatological nutrient fields. The advent of regular satellite sea surface height observations and, soon, the ARGO profiling float array provide additional information on eddy kinetic energy and thermocline structure, key for estimating subsurface nutrient and DIC inputs to the upper ocean. The incorporation of the in situ and satellite data into numerical models of low or moderate complexity will provide a foundation for interpolating between observations and deriving accurate basin-scale pCO₂ fields and air-sea fluxes.

These statistical approaches should be augmented using more mechanistic, process models to examine the cross-correlations among key physical, chemical, and biological variables. For example, 1-D studies (Keeling *et al.*, 1997) have shown that the surface concentration of oxygen, and presumably CO₂, varies with wind speed due to surface gas exchange, turbulent mixing, and biology (which is impacted by the mixing). Cross-correlation on synoptic or storm timescales that will vary regionally is significant. The eddy-resolving models together with moorings, high-resolution survey data, and surface drifters will allow for a more thorough investigation of this and other potential aliasing factors. Prognostic basin-scale biogeochemical models can also be used to construct more robust large-scale relationships of pCO₂ to other variables.

Relate observed and historical patterns and variability in pCO₂ and ancillary tracers (TCO₂, TA, O₂, nutrients, isotopic composition of these species) to the underlying biological and physical mechanisms

Prognostic models can provide consistent and complete hindcasts of three-dimensional biological and physical fields to explore dynamical relations, and through model-data evaluation improve the parameterizations of the marine carbon cycle. A number of three-dimensional marine ecosystem models are available on regional to global scales, many of them including an active carbon cycle (e.g., Six and Maier-Reimer, 1996). Only recently, however, have

these models begun to incorporate more sophisticated treatment of ecosystem dynamics beyond simple phytoplankton-zooplankton-nutrient-detritus food webs. In particular, models for the high-nitrate low-chlorophyll (HNLC) regions such as the subpolar and Equatorial Pacific and the Southern Ocean will require some treatment of iron limitation (e.g., Moore *et al.*, 2001). Calcification, nitrogen fixation, community structure, subsurface biogeochemical dynamics, and numerical advection schemes are other important concerns (Doney, 1999). Further, these models are typically either non-eddy-resolving or eddy-permitting, and at least for the near term, mesoscale eddy effects (e.g., eddy nutrient pumping) will have to be included using some form of subgrid-scale parameterization. A key aspect of the modeling component will be the ongoing evaluation and improvement of the basic ecosystem and biogeochemical model components.

A basic premise of present modeling is that physics forces ocean biogeochemistry; if we knew the physics well and had the proper ecological and biogeochemical models, we could predict large-scale biogeographic spatial patterns, the seasonal cycle, and interannual climate variability. An assumption is that intrinsic biological modes may affect individual species but do not greatly impact carbon fluxes. Getting the physics right is therefore fundamental. Physical hindcasts that cover the past several decades are becoming common (1950s to present, but with the bulk of the evaluation/forcing observations from about 1970 on). These simulations can take one of two forms: unconstrained forward models (e.g., Doney *et al.*, 2001), and state estimation/data assimilation models (e.g., Stammer *et al.*, 2001). The resulting physical fields should be used to drive simulations of pCO₂ variability in order to evaluate biogeochemical model skill, separate the relative importance of physical and biological processes on the variability of pCO₂ and ancillary tracers, and explore the response of ocean pCO₂ and other properties to regional, interannual climate modes (ENSO, PDO, NAO, etc.). As mentioned above, these simulations will also serve as the basis for surface pCO₂ extrapolation products.

Initiate surface ocean color and pCO₂ data assimilation studies

Biogeochemical data assimilation is in its infancy, and a three-phased approach is likely warranted. As outlined above, the first phase will involve assimilation of the much-better-sampled physical variables and off-line ecological and biogeochemical simulations. The second phase will include active assimilation of satellite ocean color as well as physics. The third phase will involve the assimilation of in situ pCO₂ data and other tracers such as mixed layer nutrient concentrations and biological O₂ supersaturation. This rationale is driven by the fact that a biogeochemistry model is only as good as the underlying physics and is limited by the current paucity of in situ surface pCO₂ (and related) data. At this time, the most effective strategy may be to use the emerging field data sets indirectly to improve the ecosystem and biogeochemistry models. Inversion of the subsurface carbon, nutrient, and oxygen fields is also important in that it provides complementary climatological estimates of export production and surface air-sea fluxes.

A number of recent parameter optimization studies have been conducted for marine biogeochemical box and one-dimensional models, particularly with time-series data (e.g., Mearns, 1995; Fasham and Evans, 1995; Hurtt and Armstrong, 1996; Fennel *et al.*, 2001). Applications to three-dimensional models are more limited, but include efforts to assimilate satellite ocean color data into ecosystem models (e.g., Ishizaka, 1990). Presently, the appropriate methods for assimilating biological and chemical data are an open research question, which should be explored during the initial phase of the project. The utility of data assimilation will continue to grow with the import and refinement of numerical methods from meteorology and physical oceanography to interdisciplinary problems (Robinson, 1996) and with the availability of automated software systems for generating the required model adjoints (Giering and Kaminski, 1998).

5.2.10 Modeling studies of CO₂ in the ocean interior

There are four synthesis and modeling challenges specific to the ocean interior observation component:

- Extrapolate ocean interior observations on repeat ocean transects, time-series stations, and autonomous platforms to determine the ocean carbon inventory and its changes in space and time, including interannual variability.
- Use ocean interior observations to infer air-sea fluxes of carbon and transport of carbon within the oceans, and their variability in space and time.
- Relate the observed patterns and variability of carbon and other tracers to the underlying biological mechanisms with the aim of developing improved models.
- Continue improving and assessing tracer transport characteristics in oceanic general circulation models, especially those used to diagnose carbon sources and sinks.

Extrapolate ocean interior observations to determine the ocean carbon inventory and its changes in space and time, including interannual variability

The primary aim of the ocean interior measurement program is to provide constraints on the changes in the ocean carbon inventory in space and through time. However, because of the difficulty of obtaining direct measurements, the observations are and will always be relatively sparse in space and time. Furthermore, they exhibit considerable seasonal and interannual variability. The use of such measurements to determine long-term inventory changes has thus required the development of a number of methods to determine the excess (anthropogenic) dissolved inorganic carbon either by estimating and removing the background preindustrial CO₂ field (e.g., Brewer, 1978; Chen and Millero, 1979; Goyet *et al.*, 1999; Gruber *et al.*,

1996) or computing the temporal change in ocean CO₂ directly by differencing one set of cruises and another (Wallace, 1995, 2001). Recent comparisons of methods for detecting excess dissolved inorganic carbon showed significant disagreements between different approaches (Wanninkhof *et al.*, 1999; Coatanoan *et al.*, 2001). All the methods involve assumptions that can be tested with model simulation results. A good example is the calculation of the preindustrial, dissolved inorganic carbon disequilibrium, which, if incorrect, could significantly bias the thermocline anthropogenic CO₂ estimate. Furthermore, as model simulations improve, it will be possible to use data assimilation to obtain an independent estimate of the change in inventory through time. Finally, it is important that the measurement strategy be continually tested and improved through time. Model simulations have played and will continue to play a key role in this regard.

Use ocean interior observations to infer air-sea fluxes of carbon and transport of carbon within the oceans, and their variability in space and time

Analogous to the atmospheric transport and inversion studies, the air-sea fluxes of biogeochemical species (including CO₂) can be derived in theory by inversion of interior oceanic carbon system observations using oceanic circulation and biogeochemical models (e.g., Gruber *et al.*, 2001; Gloor *et al.*, 2001). This relatively new approach in oceanography has many similarities to the atmospheric calculations, but some significant differences and unique problems as well. For example, the mixing timescale of the troposphere is only a few years; by contrast the mixing timescale of the deep ocean is several thousand years. The stability of the ocean circulation over such periods, an implicit assumption of the current inverse approach, is not well assured. The inversion of ocean interior observations has to date been conducted for a single circulation model, and considerably more work is warranted to explore the sensitivity to the physical and biogeochemical model framework, underlying assumptions and experiment formulation, and the inversion techniques. Furthermore, this work should be more closely tied to and related with more traditional box inverse models and Greens function analysis, which have been used for some time in the oceanographic community to infer ocean circulation, biogeochemical rates and transport (Schlitzer, 1999), and transient tracer uptake.

Relate the observed patterns and variability of carbon and other tracers to the underlying biological mechanisms with the aim of developing improved models

Many of the modeling issues raised with regard to surface pCO₂ apply to ocean interior CO₂ simulations as well. The subsurface distributions of CO₂, alkalinity, oxygen, and nutrients are strongly driven by the so-called biological pump, and more mechanistic parameterizations are needed for surface net community production, dissolved and particulate organic matter export fluxes, and subsurface remineralization. Despite important recent advances

in our understanding of the role of particulate as well as dissolved organic matter in the export of carbon from the surface into the ocean interior (e.g., Armstrong *et al.*, 2001; Carlson and Ducklow, 1995; Hansell and Carlson, 1998; Kirchman *et al.*, 1993), more realistic export fluxes will require better treatment of, for example, planktonic functional groups (e.g., nitrogen fixers, calcifiers), dissolved organic carbon and nutrient cycling, and mesoscale eddies. We have an even poorer understanding of the biological and physical processes that occur in the subsurface waters of the main thermocline, the so-called twilight zone, where most of exported organic matter is remineralized. The National Science Foundation has prepared plans to study these processes in future years. The interior measurements proposed in this plan will provide information on the mechanisms involved in the vertical transport, transformation, and remineralization of organic matter that will complement the proposed subsurface biogeochemical observations. Together these data will be important constraints when developing more realistic biogeochemical models as well as improved physical circulation (see the next recommendation).

Continue improving and assessing tracer transport characteristics in oceanic general circulation models, especially those used to diagnose carbon sources and sinks

The constantly varying oceanic circulation redistributes carbon horizontally and vertically, and so the synthesis and interpretation of observations require adequate representation of transport and mixing and their variations. Oceanic constituents have source/sink distributions and lifetimes different from temperature, salinity, and other traditional physical circulation parameters. Thus, simulations of tracer distributions reveal different strengths and weaknesses of the general circulation models, as amply revealed by OCMIP. In particular, the OCMIP intercomparisons reveal large discrepancies in model simulations of the vertical structure of tracers in the ocean, as discussed in the introduction to this section. Oceanic data useful for testing and improving oceanic models include the chlorofluorocarbons and radiocarbon as well as traditional hydrographic tracers and nutrient distributions.

5.2.11 Modeling studies of the global coupled carbon-climate system

There are two basic synthesis and modeling challenges specific to the global coupled carbon-climate system component:

- Improve and evaluate global coupled carbon-climate models.
- Develop techniques for carbon data assimilation into global coupled models.

Improve and evaluate global coupled carbon-climate models

The advent of global coupled carbon-climate models is a very recent advance (e.g., Cox *et al.*, 2000), and considerable effort is required to develop a robust set of models, diagnostics, and model-data evaluation metrics so that coupled models can be used with confidence for interannual variability and future climate scenarios. In addition to all of the problems associated with developing and validating the individual biogeochemical models, a number of issues arise unique to the coupled system. First, the climate of coupled physical models is typically degraded relative to either the observed state and/or uncoupled component models, which have been “tuned” to match observations (Blackmon *et al.*, 2001). The additional complexity associated with the coupled system suggests that the solutions to such problems will not be simple or direct. These physical errors will propagate through the biogeochemical and carbon systems as well. Second, the variability in the coupled solutions can only be compared with observations in a statistical sense, greatly complicating model validation exercises. Third, similar to the physical system, coupling will lead to new dynamical behaviors and model-data error patterns associated with exchanges of carbon among the reservoirs that do not occur in the uncoupled model components.

Develop techniques for carbon data assimilation into global coupled models

An ambitious program of assimilation of chemical tracer data into coupled atmosphere-land-ocean models can be envisioned in the middle of the decade. Rather than simply estimating regional surface fluxes from mass-balance considerations in a well-observed (and well-simulated) atmosphere (as outlined in the atmospheric section above), this approach would optimize parameters in underlying biogeochemical and biogeophysical models that describe the processes responsible for the fluxes. The atmospheric observations, therefore, would be used quantitatively to better constrain some of the poorly known parameters controlling regional surface CO₂ fluxes in present simulations. Such parameters might include the temperature sensitivity of soil respiration, the wind-speed dependence of the air-sea gas exchange coefficient, and the photosynthetic capacity of forest canopies. Assimilation into global coupled models would provide improved time-resolved maps of surface carbon exchange, but also lead to progressive improvements in the predictive capability of the process models over time. This kind of work has already begun for hydrological models (Land Data Assimilation System, Walker and Houser, 2001), and has been demonstrated with simple atmosphere-land biosphere models (Rayner *et al.*, 1999).

The first goal would be to better parameterize “fast” ecophysiological responses and transport processes so that the coupled assimilation system produces synoptic to seasonal CO₂ surface fluxes that match observed short-term changes in atmospheric CO₂ and that reasonably extrapolate to unobservable parts of the diurnal cycle or cloud field. The parameters in such a model would be optimized over time and space. The mass-balance analysis

would then be used to estimate the “slower” ecological components of the fluxes (due to forest regrowth, fires, harvest, etc.). In the longer term, these slow processes could be parameterized in the assimilation model as well.

As more skill with the data assimilation methods is acquired, other data constraints could be added toward the end of the decade such as terrestrial and marine biomass and productivity, in situ surface CO₂ flux estimates (e.g., from Ameriflux sites and ocean moorings, VOS and drifters). Ideally, such a coupled model with embedded biology would predict quantities that are directly observable, including temperature, wind, atmospheric CO₂, surface ocean pCO₂, and spectral radiance at the top of the atmosphere, the latter the result of the radiative interactions with vegetation, phytoplankton, and atmospheric trace gases such as CO₂ and CO. The assimilation system would then seek to minimize a generalized cost function that includes deviations of each of the predicted quantities from the actual observations stream, which would be suitably defined to include both observations made at the surface, by automated in situ sensors, and from space. Such a system would enable near-real-time analysis of the elements of the carbon cycle on land and in the oceans, and the processes that give rise to sources and sinks. It would be invaluable both for monitoring variability and for learning about the coupled Earth system. Most important, it would enable the development of falsifiable predictive models about the future behavior of the carbon cycle and the climate system.

Constructing the coupled data assimilation system described above will require either (1) convincing the major operational centers (and their sponsors) that such an expensive expansion of their mission is worthwhile; or (2) recreating the massive infrastructure and human resources currently used in those centers for the service of the carbon cycle research effort. Which of these two paths to follow is a difficult choice. Option 1 would obviously be less expensive, building on a huge, sustained, and successful ongoing program or programs. Considerable restructuring would be required at the highest levels of the weather forecasting organizations, however, which would not be easy or perhaps even desirable to accomplish. A major parallel data assimilation effort in Earth System Science would be very expensive to build, but would be more flexible and would not risk dilution or disruption of the operational infrastructure that has become so important to meteorology and commerce. Such a specialized assimilation system in parallel with the operational centers would have the tremendous luxury of being able to perform at a significant time lag, because real-time analysis or forecasts of carbon fluxes will probably never be necessary. This approach would also accommodate an observing system that includes time-consuming postprocessing of satellite imagery and sample collection for later laboratory analysis. These types of data would be impossible to process in the assimilation system if the fluxes had to be determined on an operational timetable.